

Thiamine disulfide

67-16-3 | DTXSID6046890

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 328 °C

Global applicability domain: Outside

Local applicability domain index: 5.15e-02

Confidence level: 7.14e-01

Nearest Neighbors from the Training Set

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<div>Image not found</div> <div>Auramine</div> <div>Measured: 331</div> <div>Predicted: 349</div>	<div>Image not found</div> <div>Carfentrazone-ethyl</div> <div>Measured: 353</div> <div>Predicted: 350</div>	